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Fredholm integral equation method for the integro-differential Schrödinger equation

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ABSTRACT

A new method based on the Clenshaw–Curtis quadrature for the numerical solution of the integro-differential Schrödinger equation is investigated. The method shows that it converges quickly and the truncation errors decrease faster than any power of the inverse number of the Chebyshev support points. Discretization technique is presented in detail. Accompanying C^{++} code for the Fredholm type method is available upon request.

1. Introduction

The quantum mechanical wave function of a system of particles obeys the Schrödinger wave equation. For the case of a particle in a force field $\vec{F}(\vec{r})$, where $\vec{r}$ is the position vector of the particle from the origin, the time independent form of the Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m}\nabla_{\vec{r}}^2 + V(\vec{r})\right]\Psi(\vec{r}) = E\Psi(\vec{r}), \tag{1}$$

where E is the energy of the particle, m is the mass, $\hbar$ is Planck's constant divided by 2π, $V(\vec{r})$ is the potential, so that $\vec{F}(\vec{r}) = -\vec{\nabla}(\vec{r})$, and

$$\nabla_{\vec{r}}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

is the Laplacian. In the above equation the potential is local. For a nonlocal potential, the term $V(\vec{r})\Psi(\vec{r})$ is replaced by

$$V(\vec{r})\Psi(\vec{r}) \Longrightarrow \int U(\vec{r}, \vec{r}\,')\Psi(\vec{r}\,')\mathrm{d}^3\vec{r}\,', \tag{2}$$

and the equation becomes an integro-differential equation.

Nonlocal potentials can occur in the case of the interaction of the particle with a system of particles. Examples are as follows:

- The exchange terms required for identical particles so as to obey the Pauli excursion principle, [1], lead to nonlocalities usually of a semiseparable form: In fact, the kernel k of the semiseparable form means that

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$$k(t,s)=\begin{cases}\sum_{l=1}^{\infty} f_l^{(l)}(t)g_l^{(l)}(s) & \text{if } s<t\\ \sum_{l=1}^{\infty} p_l^{(l)}(t)q_l^{(l)}(s) & \text{if } s>t.\end{cases}$$

- When explicit reference to some particles suppressed, and is replaced in terms of expressions involving integrals over Green functions between the remaining particles, [2], then the resulting nonlocal potential becomes non-semiseparable. An example given below refers to the interaction of two nucleons (protons or neutrons), mediated by the exchange of mesons, whose coordinates are suppressed.
- Phenomenological nonlocalities have also been introduced in the past to simulate effects the two cases mentioned above. A well known example in nuclear physics is the Perey–Buck nonlocality [3] used to simulate the energy dependence of an equivalent local potential which describes the scattering of an incident nucleon from a nucleus.

In many applications the potential does not depend on the choice of the direction of the axes of the coordinate system. In this case

$$V(\vec{r})=V(r),\qquad U(\vec{r},\vec{r}')=U(r,r',x),$$

where $r=|\vec{r}|$ is the length of the vector $\vec{r}$, and x is the cosine of the angle between $\vec{r}$ and $\vec{r}\,'$.

The emphasis in the present paper is to investigate under which conditions the solution of (1) in terms of the Nyström Clenshaw–Curtis quadrature is feasible. Discretization of the equation is based on Clenshaw–Curtis quadrature [4] which uses the Chebyshev polynomials $T_j(r)=\cos(j\arccos(r))$, $j=0,1,\ldots,n$, and is well suited for computing antiderivatives. This discretization, however, is different from the usual Gauss–Chebyshev quadrature (see, e.g., [5–7]) and from that of Alpert [8], Reichel [9], and Kapur and Rohklin [10]. Nyström method based on piecewise polynomials for the numerical solutions of second kind Fredholm integral equations proposed by Graham and Chandler [11], which is also different from the method presented here. Many schemes, however, exist for solving integral equations with singularities (see, for example, [8,10]) and similar techniques with ones presented here have been introduced [12–14]. Also a new and very stable method for solving the radial Schrödinger equation has been proposed recently [15,16]. The authors in above references transformed a Schrödinger differential equation into an integral equation, and then used a spectral integration technique involving Chebyshev polynomials.

In Section 2, an equivalent integral equation of (1) is discussed. A discretization technique for the integral equation is presented in detail in Section 3. Numerical examples are shown in Section 4, and summary and conclusion follow in Section 5.

2. Equivalent integral equation

In this section a transformed integral equation of the integro-differential Schrödinger equation (1) will be introduced, and then analyze it in detail using the definition given below for the discretization.

As discussed in the previous section, if there are more than two particles present, then the potentials can become nonlocal and the differential Schrödinger equation becomes an integro-differential equation for the wave function ψ,

$$\frac{\mathrm{d}^2\psi(r)}{\mathrm{d}r^2}+\kappa^2\psi(r)=\int_0^{\mathrm{T}} v(r,r')\psi(r')\mathrm{d}r', \tag{3}$$

which is defined for $0<r<\infty$, satisfies the condition $\psi(0)=0$, and is bounded at infinity. It is assumed that $v(r,r')$ is negligible for $r>T$ or $r'>T$, (see e.g. [1]). Because it is numerically more difficult to solve the Schrödinger equation in the presence of a nonlocal potential, the latter is customarily replaced by an approximate local equivalent potential. There is, however, a renewed interest in the nonlocal equations, and a significant number of papers on this subject appeared in the past few years.

Using the technique of [15,16], it is easy to show that (3) is equivalent to the following integral equation,

$$\psi(r)+\frac{\cos(\kappa r)}{\kappa}\int_0^r \sin(\kappa r')\int_0^{\mathrm{T}} v(r',p)\psi(p)\mathrm{d}p\mathrm{d}r'+\frac{\sin(\kappa r)}{\kappa}\int_r^{\mathrm{T}}\cos(\kappa r')\int_0^{\mathrm{T}} v(r',p)\psi(p)\mathrm{d}p\mathrm{d}r'=\sin(\kappa r)$$

or

$$\psi(r)+\frac{\cos(\kappa r)}{\kappa}\int_0^{\mathrm{T}} k_1(r,r')\psi(r')\mathrm{d}r'+\frac{\sin(\kappa r)}{\kappa}\int_0^{\mathrm{T}} k_2(r,r')\psi(r')\mathrm{d}r'=\sin(\kappa r), \tag{4}$$

where

$$k_1(r,r')=\int_0^r \sin(\kappa p)v(p,r')\mathrm{d}p,\qquad k_2(r,r')=\int_r^{\mathrm{T}}\cos(\kappa p)v(p,r')\mathrm{d}p.$$

Because of the characteristic of $v(p,r')$ in various potentials, the following definition is needed.

Definition 1. A kernel $k(t,s)$ is called (p_1,p_2)-semismooth, if

$$k(t,s)=\begin{cases}k_1(t,s) & \text{if } a\le s\le t\\ k_2(t,s) & \text{if } t\le s\le b,\end{cases}$$

where $k_1(t,s)\in C^{p_1}_{[a,b]\times[a,b]}$ and $k_2(t,s)\in C^{p_2}_{[a,b]\times[a,b]}$ for some $p_1,p_2>1$.

If v is semismooth, then $v(p,r')$ can be rewritten as follows,

$$v(p,r')=\begin{cases}v_1(p,r') & \text{if } 0\le p\le r'\\ v_2(p,r') & \text{if } r'\le p\le T.\end{cases}$$

In order to discretize Eq. (4) in next section, we rewrite the equation as follows,

$$\psi(r)+\frac{c(r)}{\kappa}\int_0^r k_1(r,r')\psi(r')\mathrm{d}r'+\frac{c(r)}{\kappa}\int_r^{\mathrm{T}} k_1(r,r')\psi(r')\mathrm{d}r'+\frac{s(r)}{\kappa}\int_0^r k_2(r,r')\psi(r')\mathrm{d}r'+\frac{s(r)}{\kappa}\int_r^{\mathrm{T}} k_2(r,r')\psi(r')\mathrm{d}r'=s(r), \tag{5}$$

where for notational convenience we abbreviate, $c(r)=\cos(\kappa r)$, and $s(r)=\sin(\kappa r)$. With the following notations and definitions given below,

$$k_1(r,r')=\begin{cases}k_{11}(r,r') & \text{if } 0\le r'\le r\\ k_{12}(r,r') & \text{if } 0\le r\le r',\end{cases}$$

and

$$k_2(r,r')=\begin{cases}k_{21}(r,r') & \text{if } r'\le r\le T\\ k_{22}(r,r') & \text{if } r\le r'\le T,\end{cases}$$

where

$$\begin{cases}k_{11}(r,r') &= \displaystyle\int_0^{r'} s(p)v_1(p,r')\mathrm{d}p+\int_{r'}^{r} s(p)v_2(p,r')\mathrm{d}p,\\ &= \displaystyle\int_0^{r'} s(p)v_1(p,r')\mathrm{d}p+\int_0^{r} s(p)v_2(p,r')\mathrm{d}p-\int_0^{r'} s(p)v_2(p,r')\mathrm{d}p,\\ k_{12}(r,r') &= \displaystyle\int_0^{r} s(p)v_1(p,r')\mathrm{d}p\\ k_{21}(r,r') &= \displaystyle\int_r^{\mathrm{T}} c(p)v_2(p,r')\mathrm{d}p\\ k_{22}(r,r') &= \displaystyle\int_r^{r'} c(p)v_1(p,r')\mathrm{d}p+\int_{r'}^{\mathrm{T}} c(p)v_2(p,r')\mathrm{d}p,\\ &= \displaystyle\int_r^{\mathrm{T}} c(p)v_1(p,r')\mathrm{d}p-\int_{r'}^{\mathrm{T}} c(p)v_1(p,r')\mathrm{d}p+\int_{r'}^{\mathrm{T}} c(p)v_2(p,r')\mathrm{d}p.\end{cases} \tag{6}$$

We can now rewrite Eq. (4) as follows,

$$\psi(r)+\frac{c(r)}{\kappa}\int_0^r k_{11}(r,r')\psi(r')\mathrm{d}r'+\frac{c(r)}{\kappa}\int_r^{\mathrm{T}} k_{12}(r,r')\psi(r')\mathrm{d}r'+\frac{s(r)}{\kappa}\int_0^r k_{21}(r,r')\psi(r')\mathrm{d}r'+\frac{s(r)}{\kappa}\int_r^{\mathrm{T}} k_{22}(r,r')\psi(r')\mathrm{d}r'=s(r). \tag{7}$$

3. Discretization technique

We now consider general semismooth kernels, as in Definition 1, before we discretize Eq. (7), for which we write

$$x(t)+\int_a^t k_1(t,s)x(s)\mathrm{d}s+\int_t^b k_2(t,s)x(s)\mathrm{d}s=y(t),\quad a\le t\le b. \tag{8}$$

Without loss of generality, first assume that $a=-1$, $b=1$ and let

$$F(t)=\int_{-1}^t k_1(t,s)x(s)\mathrm{d}s,\qquad G(t,\lambda)=\int_{-1}^{\lambda} k_1(t,s)x(s)\mathrm{d}s,$$

such that $F(t)=G(t,t)$, and let

$$H(t)=\int_t^1 k_2(t,s)x(s)\mathrm{d}s,\qquad J(t,\lambda)=\int_{\lambda}^1 k_2(t,s)x(s)\mathrm{d}s.$$

Further, assume that $k_1(t_k, s)x(s)$ can be expanded in a finite set of Chebyshev polynomials, i.e.,

$$k_1(t_k, s)x(s) = \sum_{i=0}^{n} \alpha_{ki} T_i(s). \tag{9}$$

If

$$G(t_k, \lambda) = \sum_{j=0}^{n+1} \beta_{kj} T_j(\lambda), \tag{10}$$

then Clenshaw–Curtis [4] showed that

$$[\beta_{k0},\ \beta_{k1}, \ldots, \beta_{kn+1}]^{\mathrm{T}} = \mathbf{S}_L\, [\alpha_{k0}, \alpha_{k1}, \ldots, \alpha_{kn}]^{\mathrm{T}}, \tag{11}$$

where

$$\mathbf{S}_L = \begin{bmatrix} 1 & 1 & -1 & 1 & \cdots & (-1)^n \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & \frac{-1}{2} & 0 & \cdots & 0 \\ 0 & \frac{1}{4} & 0 & \frac{-1}{4} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \frac{1}{2(n-1)} & 0 & \frac{-1}{2(n-1)} \\ 0 & \cdots & 0 & 0 & \frac{1}{2n} & 0 \end{bmatrix}$$

is the so called left spectral integration matrix. Here $[\nu]^{\mathrm{T}}$ denotes the transpose of the column vector ν. Similarly, assume that $k_2(t_k, s)x(s) = \sum_{j=0}^{n} \tilde{\alpha}_{kj} T_j(s)$. If

$$J(t_k, \lambda) = \int_{\lambda}^{1} k_2(t_k, s)x(s)\mathrm{d}s = \sum_{j=0}^{n+1} \tilde{\beta}_{kj} T_j(\lambda),$$

then

$$\left[\tilde{\beta}_{k0}, \tilde{\beta}_{k1}, \ldots, \tilde{\beta}_{kn+1}\right]^{\mathrm{T}} = \mathbf{S}_R \left[\tilde{\alpha}_{k0}, \tilde{\alpha}_{k1}, \ldots, \tilde{\alpha}_{kn}\right]^{\mathrm{T}}, \tag{12}$$

where

$$\mathbf{S}_R = \begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 0 & -1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & -1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & \cdots & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & \frac{-1}{2} & 0 & \cdots & 0 \\ 0 & \frac{1}{4} & 0 & \frac{-1}{4} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \frac{1}{2(n-1)} & 0 & \frac{-1}{2(n-1)} \\ 0 & \cdots & 0 & 0 & \frac{1}{2n} & 0 \end{bmatrix}$$

is the right spectral integration matrix. We want to remark that in writing the equality sign in (11) and (12), we assume that β_{n+1} and $\tilde{\beta}_{n+1}$ are set to zero. This is an acceptable assumption because in practical applications the kernel $k(t, s)$ and the r.h.s. $y(t)$ are not polynomials and the equality in (9) is only approximate. In fact, following Clenshaw and Curtis, [4], the size of α_n's and β_n's are used as a readily available tool to control the accuracy of approximation, and we chose n large enough such that α_n's and β_n's are less than a prescribed tolerance. Therefore setting β_{n+1} and $\tilde{\beta}_{n+1}$ to zero does not affect the overall accuracy.

Let τ_k, $k = 0, 1, \ldots, n$, denote the zeros of T_{n+1}. Substituting $\lambda = \tau_k$, $k = 0, 1, \ldots, n$, into (10), we obtain that

$$\begin{bmatrix} G(t_k, \tau_0) \\ G(t_k, \tau_1) \\ \vdots \\ G(t_k, \tau_n) \end{bmatrix} = \mathbf{C}\mathbf{S}_L\mathbf{C}^{-1}\mathrm{diag}(k_1(t_k, \tau_0), \ldots, k_1(t_k, \tau_n)) \begin{bmatrix} x(\tau_0) \\ \vdots \\ x(\tau_n) \end{bmatrix}$$

and, similarly,

$$\begin{bmatrix} J(t_k,\tau_0) \\ J(t_k,\tau_1) \\ \vdots \\ J(t_k,\tau_n) \end{bmatrix} = \mathbf{CS}_R\mathbf{C}^{-1}\mathrm{diag}(k_2(t_k,\tau_0),\ldots,k_2(t_k,\tau_n)) \begin{bmatrix} x(\tau_0) \\ \vdots \\ x(\tau_n) \end{bmatrix}.$$

Since $F(\tau_k) = G(\tau_k,\tau_k)$ one can get

$$\begin{aligned} F(\tau_k) &= [0,\ldots,0,1,0,\ldots,0]\,\mathbf{CS}_L\mathbf{C}^{-1}\mathrm{diag}(k_1(\tau_k,\tau_0),\ldots,k_1(\tau_k,\tau_n)) \begin{bmatrix} x(\tau_0) \\ \vdots \\ x(\tau_n) \end{bmatrix} \\ &= [w_{k0}, w_{k1},\ldots,w_{kn}]\,\mathrm{diag}(k_1(\tau_k,\tau_0),\ldots,k_1(\tau_k,\tau_n)) \begin{bmatrix} x(\tau_0) \\ \vdots \\ x(\tau_n) \end{bmatrix} \\ &= [w_{k0}, w_{k1},\ldots,w_{kn}]\,\mathrm{diag}(x(\tau_0),\ldots,x(\tau_n)) \begin{bmatrix} k_1(\tau_k,\tau_0) \\ \vdots \\ k_1(\tau_k,\tau_n) \end{bmatrix} \end{aligned}$$

where $[w_{k0},\ldots,w_{kn}]$ is the $(k+1)$-st row of the matrix $\mathbf{W} \overset{\text{def}}{=} \mathbf{CS}_L\mathbf{C}^{-1}$. We need now the following identity which can be verified by direct calculation.

Lemma 2. *Let* $\mathbf{A}$ *and* $\mathbf{B}$ *be* $n \times n$ *matrices and* $\mathbf{c} = [c_1,\ldots,c_n]^{\mathrm{T}}$. *Then* $(\mathbf{A}\circ\mathbf{B})\mathbf{c} = \mathrm{diag}(\mathbf{A}\,\mathrm{diag}(c_1,\ldots,c_n)\mathbf{B}^{\mathrm{T}})$, *where* $\mathbf{A}\circ\mathbf{B}$ *denotes the Schur product of* $\mathbf{A}$ *and* $\mathbf{B}$, $(\mathbf{A}\circ\mathbf{B})_{ij} = a_{ij}b_{ij}$, $i,j = 1,\ldots,n$.

Using this lemma one can easily find that,

$$\begin{bmatrix} F(\tau_0) \\ F(\tau_1) \\ \vdots \\ F(\tau_n) \end{bmatrix} = \mathrm{diag}(\mathbf{W}\,\mathrm{diag}(x(\tau_0),\ldots,x(\tau_n))\mathbf{K}_1^{\mathrm{T}}) = (\mathbf{W}\circ\mathbf{K}_1) \begin{bmatrix} x(\tau_0) \\ \vdots \\ x(\tau_n) \end{bmatrix}, \tag{13}$$

where $\mathbf{K}_1 = (k_1(\tau_i,\tau_j))_{i,j=0}^n$. Similarly,

$$\begin{bmatrix} H(\tau_0) \\ H(\tau_1) \\ \vdots \\ H(\tau_n) \end{bmatrix} = (\mathbf{V}\circ\mathbf{K}_2) \begin{bmatrix} x(\tau_0) \\ \vdots \\ x(\tau_n) \end{bmatrix}, \tag{14}$$

where $\mathbf{V} = \mathbf{CS}_R\mathbf{C}^{-1}$. The formulas (13) and (14) can be generalized for an interval $[a,b]$ other than $[-1,1]$ by the linear change of variables, $h(\tau) = \frac{1}{2}(b-a)\tau + \frac{1}{2}(a+b)$. Thus if $\eta_j = h(\tau_j), j = 0,1,\ldots,n$, and with the notation

$$F_a(t) = \int_a^t k_1(t,s)x(s)\mathrm{d}s, \qquad H_b(t) = \int_t^b k_2(t,s)x(s)\mathrm{d}s,$$

the followings are obtained,

$$\begin{bmatrix} F_a(\eta_0) \\ F_a(\eta_1) \\ \vdots \\ F_a(\eta_n) \end{bmatrix} = \frac{b-a}{2}(\mathbf{W}\circ\mathbf{K}_1) \begin{bmatrix} x(\eta_0) \\ x(\eta_1) \\ \vdots \\ x(\eta_n) \end{bmatrix} \tag{15}$$

and,

$$\begin{bmatrix} H_b(\eta_0) \\ H_b(\eta_1) \\ \vdots \\ H_b(\eta_n) \end{bmatrix} = \frac{b-a}{2}(\mathbf{V}\circ\mathbf{K}_2) \begin{bmatrix} x(\eta_0) \\ x(\eta_1) \\ \vdots \\ x(\eta_n) \end{bmatrix}. \tag{16}$$

Using (15) and (16) one can now discretize the Eq. (8) as follows,

$$\left[\mathbf{I}+\frac{b-a}{2}(\mathbf{W}\circ\mathbf{K}_1+\mathbf{V}\circ\mathbf{K}_2)\right]\bar{\mathbf{x}}=\bar{\mathbf{y}}, \tag{17}$$

where $\bar{\mathbf{x}}=[x(\eta_0),\ldots,x(\eta_n)]^{\mathrm{T}}$ and $\bar{\mathbf{y}}=[y(\eta_0),\ldots,y(\eta_n)]^{\mathrm{T}}$.

We now estimate the accuracy of approximation of the integral equation (8) with the linear system of Eqs. (17). The following property of Chebyshev expansions can be derived along the lines of an argument in Gottlieb and Orszag [17].

Proposition 3. *Let $f\in C^r[-1,1]$, $r>1$, and let*

$$f(t)=\sum_{j=0}^{\infty}\alpha_j T_j(t),\quad -1\le t\le 1.$$

Then

$$|\alpha_j|\le\frac{2}{\pi}\int_0^{\pi}\left|\frac{\mathrm{d}^r}{\mathrm{d}\theta^r}f(\cos\theta)\right|\mathrm{d}\theta\frac{1}{j^r}=\frac{c}{j^r}$$

and

$$\left|f(t)-\sum_{j=0}^{n}\alpha_j T_j(t)\right|\le\frac{c}{r-1}\frac{1}{n^{r-1}}.$$

It implies that if $f(r)$ is analytic then the convergence of Chebyshev expansions is super-algebraic. Let now $F_l(x)=\int_{-1}^{x}f(t)\mathrm{d}t$ and $F_r(x)=\int_x^1 f(t)\mathrm{d}t$. The following result can be found in Greengard and Rokhlin [12].

Proposition 4. *Suppose that $f\in C^r_{[-1,1]}$, $r>1$, and that $\bar{f}=(f(\tau_0),\ldots,f(\tau_n))^{\mathrm{T}}$, is the vector of the function values at the roots of $T_{n+1}(x)$. Suppose further that $\bar{F}_l$ and $\bar{F}_r$ are defined by*

$$\bar{F}_l=(F_l(\tau_0),\ldots,F_l(\tau_n))^{\mathrm{T}},\qquad \bar{F}_r=(F_r(\tau_0),\ldots,F_r(\tau_n))^{\mathrm{T}}.$$

Then

$$\|\bar{F}_l-\mathbf{C}\mathbf{S}_L\mathbf{C}^{-1}\bar{f}\|_\infty=O\left(\frac{1}{n^{r-1}}\right)$$

and

$$\|\bar{F}_r-\mathbf{C}\mathbf{S}_R\mathbf{C}^{-1}\bar{f}\|_\infty=O\left(\frac{1}{n^{r-1}}\right).$$

Furthermore, all elements of the matrix $\mathbf{C}\mathbf{S}_L\mathbf{C}^{-1}$ and $\mathbf{C}\mathbf{S}_R\mathbf{C}^{-1}$ are strictly positive.

Applying the quadrature described in above to Eq. (7), a corresponding discretized form of the equation is

$$\left[\mathbf{I}+\frac{T}{2\kappa}\mathbf{D}_c(\mathbf{W}\circ\mathbf{K}_{11}+\mathbf{V}\circ\mathbf{K}_{12})+\frac{T}{2\kappa}\mathbf{D}_s(\mathbf{W}\circ\mathbf{K}_{21}+\mathbf{V}\circ\mathbf{K}_{22})\right]\bar{\psi}=\bar{\mathbf{s}}, \tag{18}$$

where in more detail,

$$\begin{cases}
\bar{\psi}=[\psi(t_0),\psi(t_1),\ldots,\psi(t_n)]^{\mathrm{T}},\\
\mathbf{D}_c=\mathrm{diag}(\cos(\kappa t_0),\cos(\kappa t_1),\ldots,\cos(\kappa t_n)),\\
\mathbf{D}_s=\mathrm{diag}(\sin(\kappa t_0),\sin(\kappa t_1),\ldots,\sin(\kappa t_n)),\\
\bar{\mathbf{s}}=[\sin(\kappa t_0),\sin(\kappa t_1),\ldots,\sin(\kappa t_n)]^{\mathrm{T}},\\
\mathbf{W}=\mathbf{C}\mathbf{S}_L\mathbf{C}^{-1},\qquad \mathbf{V}=\mathbf{C}\mathbf{S}_R\mathbf{C}^{-1},\\
\mathbf{K}_{11}=(k_{11}(t_i,t_j))_{i,j=0}^{n}\\
\quad=\dfrac{T}{2}[(\mathbf{W}\mathbf{D}_s(\mathbf{V}_1-\mathbf{V}_2))_{jj}+(\mathbf{W}\mathbf{D}_s\mathbf{V}_2)_{ij}]\\
\mathbf{K}_{12}=(k_{12}(t_i,t_j))_{i,j=0}^{n}\\
\quad=\dfrac{T}{2}(\mathbf{W}\mathbf{D}_s\mathbf{V}_1)_{ij},\\
\mathbf{K}_{21}=(k_{21}(t_i,t_j))_{i,j=0}^{n},\\
\quad=\dfrac{T}{2}(\mathbf{V}\mathbf{D}_c\mathbf{V}_2)_{ij}\\
\mathbf{K}_{22}=(k_{22}(t_i,t_j))_{i,j=0}^{n}\\
\quad=\dfrac{T}{2}[(\mathbf{V}\mathbf{D}_c\mathbf{V}_1)_{ij}+(\mathbf{V}\mathbf{D}_c(\mathbf{V}_2-\mathbf{V}_1))_{jj}].
\end{cases} \tag{19}$$

If the kernel $k(t,s)$ depends on the difference of the arguments,

$$k(t,s) = k(|t-s|) = \begin{cases} k_1(t,s) & \text{if } a \le s \le t \\ k_2(t,s) & \text{if } t \le s \le b, \end{cases}$$

and if we use a uniform partition with the same number of points per partition, then $k_r(\tau_p^{(i)}, \tau_q^{(i)}) = k_r(\tau_p, \tau_q), r = 1, 2$, where $\tau_p^{(i)}$ and $\tau_q^{(i)}$ are the support points in i-th subinterval of $b_1 = 0 \le b_2 \le \cdots \le b_{i-1} \le b_i \le \cdots T = b_m$, and Eq. (18) becomes a block Toeplitz matrix,

$$\begin{bmatrix} \mathbf{A}_1 & \tilde{\mathbf{A}}_2 & \tilde{\mathbf{A}}_3 & \cdots & \tilde{\mathbf{A}}_m \\ \mathbf{A}_2 & \mathbf{A}_1 & \tilde{\mathbf{A}}_2 & \cdots & \tilde{\mathbf{A}}_{m-1} \\ \mathbf{A}_3 & \mathbf{A}_2 & \mathbf{A}_1 & \cdots & \tilde{\mathbf{A}}_{m-2} \\ & \ddots & \ddots & \ddots & \\ \mathbf{A}_m & \mathbf{A}_{m-1} & \cdots & \mathbf{A}_2 & \mathbf{A}_1 \end{bmatrix} \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_m \end{bmatrix} = \begin{bmatrix} \bar{y}_1 \\ \bar{y}_2 \\ \vdots \\ \bar{y}_m \end{bmatrix}, \tag{20}$$

where

$$\mathbf{A}_1 = \left[\mathbf{I} + \frac{b_i - b_{i-1}}{2} (\mathbf{W} \circ \mathbf{K}_1^{(i)} + \mathbf{V} \circ \tilde{\mathbf{K}}_2^{(i)}) \right],$$

$$\mathbf{A}_i = \frac{b_i - b_{i-1}}{2} [(\mathbf{W} + \mathbf{V}) \circ \mathbf{K}_2^{(i)}], \quad i \ne 1$$

$$\tilde{\mathbf{A}}_i = \frac{b_i - b_{i-1}}{2} [(\mathbf{W} + \mathbf{V}) \circ \mathbf{K}_1^{(i)}], \quad i \ne 1$$

with $\mathbf{K}_2^{(i)} = k_2(\tau_j^{(i)}, \tau_k^{(i)}) = k_2(\tau_j, \tau_k)$ and $\mathbf{K}_1^{(i)} = k_1(\tau_j^{(i)}, \tau_k^{(i)}) = k_1(\tau_j, \tau_k)$. The Toeplitz system of equations can be efficiently solved by the iterative conjugate gradients methods in $O(m \log(m))$ arithmetic operations, or by direct divide-and-conquer type algorithms in $O(m \log^2(m))$ arithmetic operations, or by direct Levinson type algorithm in $O(m^2)$ arithmetic operations. Each of these techniques has its uses, depending on the properties of the Toeplitz matrix and the underlying science model. References to Toeplitz solvers can be found, for example, in an expository paper by Chan and Ng [18].

4. Numerical examples

We illustrate now the obtained discretization with examples. The number of points used in discretizations is denoted by n. *Error* denotes $\|x - x_\tau\|_\infty / \|x\|_\infty$, where x and x_τ are the analytic and the numerical solutions, respectively. In each plot, $\log(Error)$ is the common logarithm of the *Error*. All computations were done on a personal computer with operating system CentOs Linux in double precision. We remark that the values of $x(t)$ are found inside the interval (or each of the subintervals of partition) at Chebyshev points $\tau_0, \tau_1, \ldots, \tau_n$. The value of $x(t)$ for $t \ne \tau_k$ can be found as follows. Applying $\mathbf{C}^{-1}$ we can find "Chebyshev–Fourier" coefficients of $x(t)$,

$$\begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix} = \mathbf{C}^{-1} \begin{bmatrix} x(\tau_0) \\ x(\tau_1) \\ \vdots \\ x(\tau_n) \end{bmatrix}.$$

Thus,

$$x(t) \cong \sum_{j=0}^{n} \alpha_j T_j(h(t)), \quad a \le t \le b.$$

The value of $T_j(t)$ for $t \ne \tau_k$ is found now using the recursion satisfied by Chebyshev polynomials, $T_{j+1}(t) = 2tT_j(t) - T_{j-1}(t)$.

In Example 1, we use a prototype of the Yukawa potential, (see, e.g., [19], 23.c), which is simplified to a degree such that an analytic solution can be found. In our terminology this potential is semiseparable. We note once more that the case of this semi-separable potential could be also treated by the techniques already presented in [15], and we use it here only because the comparison with the analytic solution is possible.

Example 1. Let

$$v(p, r') = \begin{cases} \lambda e^{p - r'} & \text{if } 0 \le p \le r' \\ \lambda e^{r' - p} & \text{if } r' \le p \le T. \end{cases}$$

It is easy to see that if $\psi(r) = e^{-r}$, then the right-hand side has the form,

$$y(r) = \left(1 - \frac{3\lambda\kappa}{4}\right) e^{-r} + \frac{3\lambda\kappa}{4} \cos(r) - \frac{\lambda\kappa}{2} r e^{-r}.$$

Table 1
$T = 20$, $\kappa = 1$ and $\lambda = 0.1$

n	16	32	64	128	256
Error	1.2e+01	3.4e−07	8.1e−09	3.4e−09	6.0e−09

Table 2
$T = 20$, $A = 100$, $\kappa = 1$ and $\lambda = 0.1$

n	8	16	32	64	128	256
e_n	1.0e−0	1.2e−03	1.6e−09	7.7e−15	1.6e−14	4.8e−14

By comparing the analytical solution given above with the numerical solution of (18) at the discretization points, we get the relative errors as given in Table 1, in the case of $\lambda = 0.1$, $\kappa = 1$ and $T = 20$.

In the second example we consider a more interesting case for which the techniques of [15] are not applicable. This time the non-locality is a prototype of the optical model Perey–Buck potential [3]. In our terminology this potential is semi-smooth, but not semiseparable.

Example 2. Let

$$v(p, r') = \frac{\lambda e^{-\frac{|r'-p|}{A}}}{1 + e^{-\frac{|r'-p|}{A}}} = \begin{cases} \dfrac{\lambda e^{\frac{p-r'}{A}}}{1 + e^{\frac{p-r'}{A}}} & \text{if } 0 \le p \le r' \\ \dfrac{\lambda e^{\frac{r'-p}{A}}}{1 + e^{\frac{r'-p}{A}}} & \text{if } r' \le p \le T. \end{cases}$$

Since there is no analytic solution for the given $v(p, r')$ with the r.h.s $y(r) = \sin(r)$, a relative error e_n for the different number of support points is evaluated as follows; Solving (18) first at n shifted Chebyshev support points $t_i^{(n)}$, $i = 1, \ldots, n$, and $2n$ points $s_i^{(2n)}$, $i = 1, \ldots, 2n$, we, then, obtain the numerical solutions $\psi^{(n)}(r)$ and $\psi^{(2n)}(r)$, respectively. Then to get the values of $\psi^{(2n)}(r)$ at $t_i^{(n)}$, we follow the procedure described in the right above Example 1. Finally The error e_n can be calculated by comparison of the solutions $\psi^{(n)}$ and $\psi^{(2n)}$ at t_i, $i = 1, 2, \ldots, n$ (see Table 2),

$$e_n = \|\psi^{(2n)}(t_i^{(n)}) - \psi^{(n)}(t_i^{(n)})\|_\infty / \|\psi^{(2n)}(t_i^{(n)})\|_\infty.$$

Here we take $\lambda = 0.1, \kappa = 1,\ A = 100$, and $T = 20$.

We see that for this choice of λ the discrete equations well conditioned and the double precision accuracy is obtained with 64 points.

In the third and fourth examples we consider a more difficult case which models the nonlocalities corresponding to a nucleon-nucleon interaction (see, e.g., [20,22]). The kernel $k(r, r')$ is propagated by logarithmic singularity. This occurs when the integration variable r'' sweeps over the region which surrounds r'. One finds that when both r and r' are close to zero, the singularity of $k(r, r')$ is proportional to $k(r, r') \propto (r - r')^2 \ln|r - r'|$, and when both r and r' are not close to the origin, the singularity is $k(r, r') \propto |r - r'| \ln|r - r'|$. The presence of this singular behavior affects the spectral accuracy of the method which is based on Clenshaw–Curtis quadrature. Our Nyström type method now gives only a single precision accuracy.

Example 3. Let $k(r, r') = (p - r')^2 \ln((p - r')^2) e^{-|p-r'|} e^{-(p+r')}$. The right-hand side is chosen to be $y(r) = \sin(r)$. Note that the right hand side is bounded and does not approach zero at infinity, which is typical for nuclear scattering applications. We use $T = 14$ and $k = 1$. The best accuracy of our algorithm is achieved for the choice of 64 partitions with 32 points per partition with the error of 5.88e−07.

The second and third columns of Table 3 show the numerical values of $\psi^{(2n)}(t_i)$ and $\psi^{(n)}(t_n)$ at t_i, $i = 1, 2, \ldots, n$, as described in Example 2, respectively.

Example 4. Let

$$k(r, r') = |p - r'| \ln((p - r')^2) e^{-|p-r'|} e^{-(p+r')}.$$

The right-hand side is chosen to be $y(r) = \sin(r)$, and we use $T = 10$ and $k = 1$ (Table 4). Again, the best accuracy of our algorithm with a personal computer is achieved for the choice of 32 partitions with 32 points per partition with the error of 8.52e−05.

Table 3
$T = 14$, and $k = 1$

Support points	Numerical solutions (2N)	Numerical solutions (N)
2.6349e−04	9.0186503677216045e−03	9.0186475215332969e−03
2.36764e−03	1.1066062742162354e−02	1.1066059882386542e−02
1.65598e−01	1.4630969265771104e−01	1.4630960182573696e−01
5.62722e−01	3.1576870575765326e−01	3.1576852701593888e−01
1.00022e+00	3.2477450202954367e−01	3.2477431691948211e−01
2.00085e+00	1.2843959331941765e−01	1.2843952756384486e−01
3.00583e+00	4.4565741993876379e−03	4.4565746148047224e−03
4.00935e+00	−1.6117316483516372e−02	−1.6117309936034965e−02
5.02052e+00	−6.8704275923111681e−03	−6.8704233813700272e−03
6.01871e+00	−5.7661391734702236e−04	−5.7661380202913496e−04
7.00026e+00	7.1717291244986303e−04	7.1717286497533243e−04
8.00022e+00	3.6701769415906809e−04	3.6701747772322288e−04
9.00085e+00	5.0174576877215679e−05	5.0174552533542233e−05
1.00058e+01	−2.9657750494892937e−05	−2.9657745403255617e−05
1.10093e+01	−1.8496471972426277e−05	−1.8496464700419689e−05
1.20205e+01	−3.1874594689731082e−06	−3.1874576045410736e−06
1.30187e+01	1.1930583581245784e−06	1.1930579652838724e−06
1.39997e+01	9.0730019145067546e−07	9.0730015872899120e−07

Table 4
$T = 10$, and $k = 1$

Support points	Numerical solutions (2N)	Numerical solutions (N)
1.882100e−04	8.5774554392600219e−03	8.5774178182761833e−03
1.691170e−03	1.0364720627537001e−02	1.0364650832259245e−02
8.944452e−02	1.1616786971381182e−01	1.1615992749990162e−01
9.888189e−01	1.2087482092366120e+00	1.2086732938664353e−01
1.499328e+00	1.4768491365210255e+00	1.4767683567855363e+00
2.008323e+00	1.3701384174781985e+00	1.3700199794879546e+00
2.500188e+00	9.3267770832053298e−01	1.2843952756384486e−01
3.006716e+00	2.0639666734406972e−01	2.0638035037295333e−01
3.134134e+00	6.1223177973244074e−03	6.1220199548020189e−03
3.140002e+00	−2.6068588664747709e−03	−2.6068748369820023e−03
4.011181e+00	−1.1802243684675320e+00	−1.1801634307641112e+00
5.000188e+00	−1.5201438560135743e+00	−1.5201056015680332e+00
6.000672e+00	−4.3304100436265547e−01	−4.3300966747841518e−01
7.008323e+00	1.0174791772727692e+00	1.0173900882373863e+00
8.006716e+00	1.4708864723964850e+00	1.4707748058590260e+00
9.011181e+00	5.1489048035388363e−01	5.1486975093375476e−01
9.999812e+01	−6.7433537494462181e−01	−6.7432689241703314e−01

5. Summary and conclusions

We describe a new accurate discretization technique for integro-differential Schrödinger equations whose kernels of integral part can be discontinuous along the main diagonal. For a semismooth kernel, it gives a much higher accuracy than was ever possible with standard Gauss type quadrature rules. It is also of comparable accuracy with Gauss type quadratures for the Volterra and the Fredholm integral equation of the second type with smooth kernels. The discretization technique can be adopted to exploit additional structure of the kernel such as a low semi-rank, or a displacement structure, $k(t, s) = k(|t - s|)$, for example, to allow for reduced complexity algorithms for the discretized equations.

The method can be applied to the quantum mechanical atomic and nuclear physics problems, where the requirement of indistinguishability of the electrons leads to nonlocalities in the potential contained in the Schrödinger equation due to the presence of exchange terms (see, e.g., [21]). We plan also to apply the discretization technique presented in this article to the scattering problem in Eddington approximation (see, e.g., [22–25]) and compare it with some of the existing methods in near future.

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